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## **S4.1**

### **Integrated modelling for assessing the risk of groundwater contaminants to human health and surface water ecosystems**

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**Abstract** The practical implementation of the European Water Framework Directive has resulted in an increased focus on the groundwater-surface water interaction zone. A gap exists with respect to preliminary assessment methodologies that are capable of evaluating and prioritising point sources of contamination. In particular, adaptive management tools designed to work with sparse data sets from preliminary site assessments are needed which can explicitly link contaminant point sources with groundwater, surface water and ecological impacts. Here, a novel integrated modelling approach was employed for evaluating the impact of a TCE groundwater plume, located in an area with protected drinking water interests, to human health and surface water ecosystems. This is accomplished by coupling the system dynamics-based decision support system CARO-Plus to the aquatic ecosystem model AQUATOX via an analytical volatilisation model for the stream. The model is tested on a Danish case study involving a 750 m long TCE groundwater plume discharging into a stream. The initial modelling results indicate that TCE contaminant plumes with  $\mu\text{g L}^{-1}$  concentrations entering surface water systems do not pose a significant risk to either human or ecological receptors.

**Key words** groundwater-surface water interfaces; integrated modelling; system dynamics; contaminated sites; uncertainty

## **INTRODUCTION**

Due to increasing global exploitation of both stream water and groundwater resources, a better awareness of the connections between these two systems and the roles they play in maintaining water quality is essential, as well as on how human activities may impair them. In recognition of this, implementation of the Water Framework Directive within the individual countries necessitates the evaluation of all types of contamination sources within a specific watershed in order to assess their direct impact on water quality and ecosystem health. Chlorinated solvents, such as trichloroethylene (TCE), and pesticides are among the most prevalent and serious contaminants of surface and groundwater resources in the world (e.g. Winter et al., 1998). In Denmark this is a major problem because almost all drinking water comes directly from groundwater (Henriksen et al., 2008). Due to their widespread use, mobility and persistence,

chlorinated volatile organic compounds (VOCs) are considered to have the greatest potential to discharge to surface waters (Ellis and Rivett, 2007). This paper focuses on the ecological impact of VOCs, specifically those discharging to streams from point sources in groundwater.

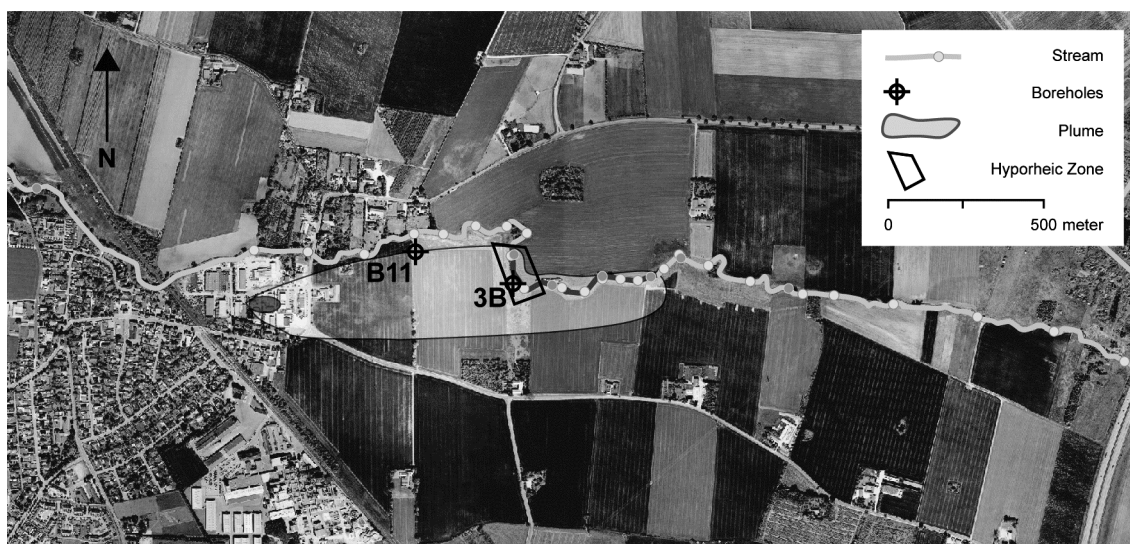
## MODELLING STUDY

### Modelling approach

An integrated modelling approach was used to support both the human health and ecological risk assessment for TCE at this site. This was accomplished by coupling the system dynamics-based decision support system CARO-Plus (Serapiglia et al., 2005; McKnight and Finkel, 2008) to the process-based aquatic ecosystem model AQUATOX (Park et al., 2008) via a simple analytical volatilization model, which could be shown to be the dominant removal process in the stream at this site (see McKnight et al., 2010).

### Case study site

The aquifer at Skensved is contaminated by TCE originating from an auto lacquer shop, which has used the solvent for degreasing metal parts since 1974. A leaking storage tank was found in 1993 where TCE had been seeping directly into the ground below, with a plume extending up to 1000 m (see Fig. 1). Although little data exists regarding the source zone, measured TCE concentrations (in the  $\text{mgL}^{-1}$  range) reveal the presence of separate phase of contaminant and show that the source will not be depleted for many decades (McKnight et al., 2010). The TCE plume is currently under hydraulic control through the implementation of pump-and-treat (GEO, 2009).



**Fig. 1** Propagation of the TCE contaminant plume at the Skensved site (McKnight et al., 2010).

## RESULTS

### Impact of TCE on Skensved stream

This section shall summarize previous findings from McKnight et al. (2010), which was focused on TCE. Volatilization was found to rapidly attenuate TCE concentrations in the surface water. Thus, only a 300 m stream reach failed to meet surface water quality criteria. A human health risk assessment of surface water found no risk for the developed worst-case scenario, i.e. children in a recreational setting. Risk was only found to exist if the groundwater was to be used as drinking water. An ecological risk assessment found that the TCE contamination does not impact the stream ecosystem.

### Impact of VOCs

In order to generalise the findings in the case study, the study was extended to additional volatile organic compounds, see Table 1, for a range of contaminant concentration scenarios (indicative for different flow conditions). Starting from the point source discharge of  $15 \text{ g d}^{-1}$  (e.g. predicted for TCE) in surface water, the concentrations were then increased (or decreased) by factors of ten in order to determine the “threshold” at which toxicant stress could perturb the AQUATOX ecosystem model.

**Table 1** Physico-chemical and ecotoxicological parameters for the organic contaminants.

Parameter	Benzene	TCE	PCE	Naphthalene
Molecular weight [g/mol]	78.12	131.39	165.83	128.17
Solubility [mg/L]	1790	1280	206	31
Log Kow [-]	2.13	2.42	3.4	3.3
Kp sediment [L/kg]*	146	253	1610	1333
Vapor pressure [mm Hg]	94.8	69.0	18.5	0.085
Henry constant – 15 deg. C [ $\text{atm} \cdot \text{m}^3/\text{mol}$ ]	0.0037	0.00615	0.01135	0.000395
LC50 Chironomid, 48 hr acute test [ $\mu\text{g/L}$ ]	34000	42000	14169**	2810
LC50 Minnow, 48 hr acute test [ $\mu\text{g/L}$ ]	12500	52000	10800	1990

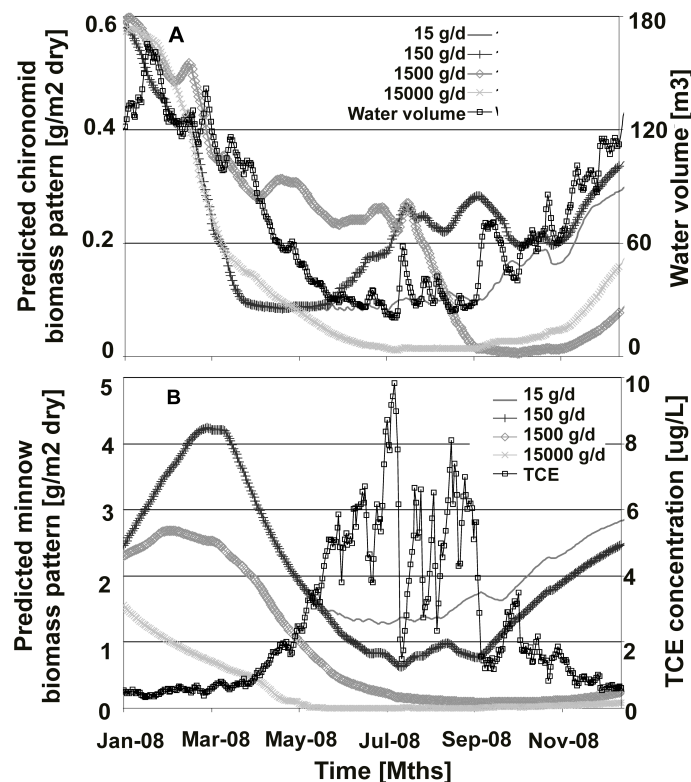
\*Calculated dynamically by AQUATOX using Log Kow, pH and pka.

\*\*Calculated by AQUATOX, regression using *D. magna*.

Figure 2 illustrates the modelling results for predicted biomass patterns for (A) chironomid (benthic invertebrate) and (B) minnow (representative fish species). For the base case scenario ( $15 \text{ g d}^{-1}$ ), water volume was found to be the limiting factor most influencing the biomass concentration. Results for the perturbed and control scenarios were identical. A clear threshold value could be determined for chironomid at  $1500 \text{ g d}^{-1}$ , whereas the minnow was already impacted at  $150 \text{ g d}^{-1}$ . Interestingly, at  $150 \text{ g d}^{-1}$ , the simulated chironomid actually increases during high TCE concentration exposure, e.g. most likely due to decreased predation.

Similar figures were created for tetrachloroethylene (PCE), benzene and naphthalene (data not shown). PCE and benzene produced comparable results to that of TCE, the only notable exception being that for benzene, the clear threshold for chironomid occurred first at  $15,000 \text{ g d}^{-1}$ . For naphthalene, the results were simply shifted one order of magnitude smaller, i.e.  $1.5 \text{ g d}^{-1}$  produced results similar to TCE base case results ( $15 \text{ g d}^{-1}$ ) and the threshold value could be found already at  $150 \text{ g d}^{-1}$ . Sensitivity analyses point to the importance of the parameter Kp sediment (see Table 1) especially for sediment feeders (e.g. chironomid), as well as the ecotoxicology parameter LC50, which determines the concentration at which mortality for 50% of the species occurs. Additional physico-chemical properties, such as lower vapour pressure

and lower solubility, most likely explain the increased ecosystem sensitivity towards the compound naphthalene.



**Fig. 2** Predicted biomass patterns for (A) chironomid and (B) minnow over time for four TCE concentration scenarios. Note that in (A) water volume and (B) TCE concentration is shown on the right-hand y-axis.

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